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Research Paper

Investigation of Electrical and Thermal Properties of Perovskite Solar Cells Through Multidimensional Simulations to Enhance Performance and Stability

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Abstract

Perovskite solar cells (PSCs) have gained widespread attention due to their impressive power conversion efficiency (PCE), low manufacturing costs, and versatile design potential. However, challenges such as thermal instability, material degradation, and inefficient charge carrier transport have limited their broader application. This research addresses these issues by investigating the electrical and thermal properties of PSCs through comprehensive 1D, 2D, and 3D simulations using COMSOL Multiphysics. The simulated solar cell structure consists of fluorine-doped tin oxide (FTO) as the front contact, titanium dioxide (TiO_2) as the electron transport layer (ETL), cuprous oxide (Cu_2O) as the hole transport layer (HTL), methylammonium lead iodide ($MAPbI_3$) as the perovskite absorber, and gold (Au) as the back contact. The 1D simulations revealed variations in energy levels, carrier concentrations, and electric potential, affecting charge transport and recombination. I-V characteristics showed a peak current density of 20.8 mA/cm² at 0.01 V, decreasing as the voltage increased to 1.2 V. The 2D simulations provided insights into the electric field distribution, with a peak field intensity of 9.64×10^6 V/m. Thermal effects were also analyzed, with a maximum nonradiative recombination heating of -3.46×10^8 W/m³. The 3D simulations offered a detailed view of charge accumulation, energy alignment, and thermal management. The analysis provides valuable insights into charge accumulation, energy level alignment, and thermal management, enabling improved device development and material characteristics. By enhancing charge separation and improving thermal stability, this research demonstrates improved performance, offering guidance for future PSC innovations.

1. Introduction

PSCs have become significant in PVs due to their exceptional combination of low production costs, high performance, and a wide range of application possibilities. PSCs have advanced quickly because of their unique material features, which include long carrier diffusion lengths, variable bandgaps, and high absorption coefficients. These features make PSCs beneficial in several kinds of renewable energy applications (Lin et al., 2017; Yamaguchi et al., 2021; Jeon et al., 2014). However, in order to properly utilize PSCs, it is essential to understand the complex interactions between thermal and electrical properties within the cell, as these variables have a significant impact on the stability and performance of the device (Zhou et al., 2021; Bi et al., 2016; Yang et al., 2016). Maintaining control over the electric field, carrier concentrations, and heat distribution within the device is one of the key challenges in PSC optimization. Understanding the complex physical processes implementing place within several dimensions calls for modeling methodologies that are meticulous. It has become increasingly important in these circumstances to use numerical simulation tools like COMSOL Multiphysics. Through solving coupled differential equations describing these phenomena, COMSOL Multiphysics facilitates a detailed study of the spatial distribution of electrical and thermal properties in PSCs (Im et al., 2014; Green et al., 2024). Researchers can obtain insights into the internal behavior of PSCs by 1-D, 2-D, and 3-D simulations, which are not easily accessible through experimental methods alone (Burschka et al., 2013; Ball et al., 2013; Wang et al., 2020).

According to recent studies, the variation of energy levels, carrier concentrations, and electric potentials along the depth of the solar cell can be accurately modeled by 1-D simulations in COMSOL Multiphysics (Zhang et al., 2022; Niu et al., 2015; Snaith, 2013). Since these locations directly affect the performance of the cell, these simulations are especially useful in finding areas of charge accumulation and depletion. Researchers can improve charge separation and develop improved PCEs by optimizing the distribution of the electric field throughout the cell. The capacity of 1-D simulations to capture lateral effects and spatial variations in the cell's plane is restricted, despite the fact that they offer insightful information about the depth profile of the cell (Habisreutinger et al., 2014; Stranks et al., 2013; Li et al., 2019). In order to overcome these constraints, the lateral distribution of electric fields and thermal characteristics inside PSCs are investigated using 2-D simulations. Through these simulations, the impact of in-plane variations on device performance—such as non-uniformities in material characteristics or fabrication defects—can be better understood (Jiang et al., 2021; Eperon et al., 2014). Furthermore, important regions of the cell that are vulnerable to energy loss as a result of phenomena like nonradiative recombination and joule heating can be identified using 2-D simulations. Comprehending these impacts is crucial in order to optimize PSC thermal management, which in turn is necessary to sustain device stability in operational conditions (Rehman et al., 2017; Seo et al., 2017; Liu et al., 2019). 3D simulations offer a comprehensive spatial representation of the electric and thermal fields within the cell, enhancing the analysis established by the insights gained from 1D and 2D simulations. These simulations enable a clearer understanding of the complex interactions among different cell regions, allowing for the identification of areas that may contribute to thermal

degradation or other performance issues (Brenner et al., 2016; Zhao et al., 2020). Researchers are advancing the development of more efficient and stable PSCs by exploring how different cell designs and material compositions affect overall device performance using 3D simulations in COMSOL Multiphysics (Conings et al., 2015; Wu et al., 2018; Bati et al., 2023). Miyasaka et al. were pioneers in introducing PSCs based on $MAPbI_3$, presenting them as a highly promising solution for PV applications (Kojima et al., 2009). Zhang et al. emphasized that the structural versatility and compositional flexibility of PSCs further enhance their potential as next-generation PV devices (Liu et al., 2021). However, Kahandal et al. examine various aspects of PSCs, including their fundamental properties, challenges related to stability, and future prospects. Their paper discusses the rapid advancements in PSC technologies, improvements in efficiency, and the challenges of thermal instability and material degradation (Kahandal et al., 2024). Rao et al. provide a comprehensive review of the persistent challenges regarding the stability of PSCs, focusing on factors such as moisture sensitivity, thermal instability, and material degradation over time (Rao et al., 2021). Elangovan et al. explore recent advancements in perovskite materials, highlighting enhancements in fabrication techniques, band gap engineering, and strategies to improve the stability of PSCs (Kumar et al., 2024). Zandi et al. investigated the numerical simulation of heat distribution in RGO-contacted perovskite solar cells using COMSOL (Zandi et al., 2020). Kumar et al. (2024) explored the effect of a 2D perovskite layer and multivalent defects on the performance of 3D/2D bilayered perovskite solar cells using simulation techniques. The results demonstrate that a thin 2D perovskite layer contributes to long-term stability by shielding the 3D perovskite, while the presence of multivalent defects in the 3D layer leads to a 4.2% decrease in efficiency. This study underscores the potential of mixed-dimensional perovskites in enhancing both the stability and efficiency of PSCs (Kumar et al., 2021). Li et al. investigate the role of mixed-dimensional integration in PSCs, analyzing the influence of 0D, 1D, 2D, and 3D structures on the performance and stability of these devices. The authors also discuss the intricate balance between material properties, device architecture, and fabrication techniques, offering essential insights for the advancement of high-performance PSCs (Li et al., 2024). Kim et al. (2023) provide a comprehensive review on the progress of 2D and 2D-3D mixed-halide perovskite materials for photovoltaic applications, emphasizing their optoelectronic characteristics and inherent challenges. The review also delves into the distinctive structural and material properties of these multidimensional perovskite systems, offering insights into their potential for future solar cell technologies (Kim et al., 2021). These simulations offer crucial insights into charge transport, energy level alignment, and heat distribution, which are essential for identifying charge accumulation and recombination zones. Such findings are vital for improving PSC performance by developing charge separation and electric field distribution, thereby guiding future enhancements in device architecture and material engineering.

This investigation centers on a point-by-point investigation of the electrical and thermal characteristics of PSCs utilizing 1D, 2D, and 3D simulations conducted with COMSOL Multiphysics. The study investigates energy levels, carrier concentrations, and electric potentials across various dimensional frameworks to reveal charge accumulation, depletion regions, and

electric field distributions that affect device performance. Additionally, it explores the spatial distribution of electric fields, thermal impacts, nonradiative recombination, and Joule heating to identify mechanisms of energy loss. The findings aim at the development of PSC design and material properties, ultimately enhancing their performance, stability, and commercial feasibility.

2. Materials and Methods

2.1 Simulations Using COMSOL Multiphysics

We performed 1-D, 2-D, and 3-D simulations of the PSC structure using COMSOL Multiphysics in order to obtain a better understanding of the spatial distribution of electrical and thermal properties. To account for the spatial differences in energy levels, carrier concentration, and electric potential, the simulation geometry was constructed for 1-D, 2-D, and 3-D scenarios, as we discussed in the result and discussion section.

2.1.1. Material Properties and Geometry:

FTO is selected for the front contact layer due to its high transparency to visible light and excellent electrical conductivity, which significantly enhance charge transport efficiency (Yao et al., 2020). TiO_2 is selected as the ETL because of its high electron mobility and suitable energy level alignment with the perovskite layer, thereby improving electron extraction (Kumar et al., 2023). Cu_2O is selected as the HTL due to its effective p-type conductivity and compatibility with $MAPbI_3$, which facilitates efficient hole transport (Zhou et al., 2020). $MAPbI_3$ is selected as the perovskite absorber layer for its high absorption coefficient and optimal bandgap, maximizing light harvesting capabilities (Targhi et al., 2018). Au is selected for the back contact because of its excellent electrical conductivity and stability, ensuring reliable charge collection (Khan et al., 2024). The materials FTO, TiO_2, Cu_2O, $MAPbI_3$, and Au were selected for their established efficacy in PSCs. While alternatives like ITO, SnO_2, and spiro-OMeTAD are available, these materials were preferred for their proven reliability, cost-effectiveness, and compatibility with the PSC structure. Fig. 1 illustrates the PSC structure along with its layer parameters for the COMSOL Multiphysics software, while Table 1 presents the component characteristics necessary for simulating the program within the COMSOL Multiphysics software (Minbashi & Yazdani, 2022).

2.1.2. Simulation Parameters:

The applied voltage (V_app) of 1.2 V was chosen to simulate the current-voltage (I-V) characteristics of the solar cell. In addition, the model incorporated heat sources, nonradiative recombination heating, joule heating, and the distribution of the electric field to accurately capture the thermal and electrical dynamics of the solar cell.

2.1.3. Equations and Models Used:

Maxwell's equations were utilized to determine the electric field (V/m):

$$\nabla \times E = -\partial B/\partial t \quad \text{.....(1)}$$

$\nabla \cdot D = \rho$ .....(2)

In this case, ρ is the charge density, D is the electric displacement field, B is the magnetic flux density, and E is the electric field.

The temperature dissemination inside the solar cell is depicted by the heat equation: $\rho c_p \partial T/\partial t = \nabla \cdot (k \nabla T) + Q$.....(3)

Where Q is the heat source term, which incorporates commitments from nonradiative recombination and joule heating, ρ is the density, c_p is the particular heat, T is the temperature, and k is the thermal conductivity (Hägglund, 2022; Song & Meng, 2013; Saxena & Gorji, 2019).

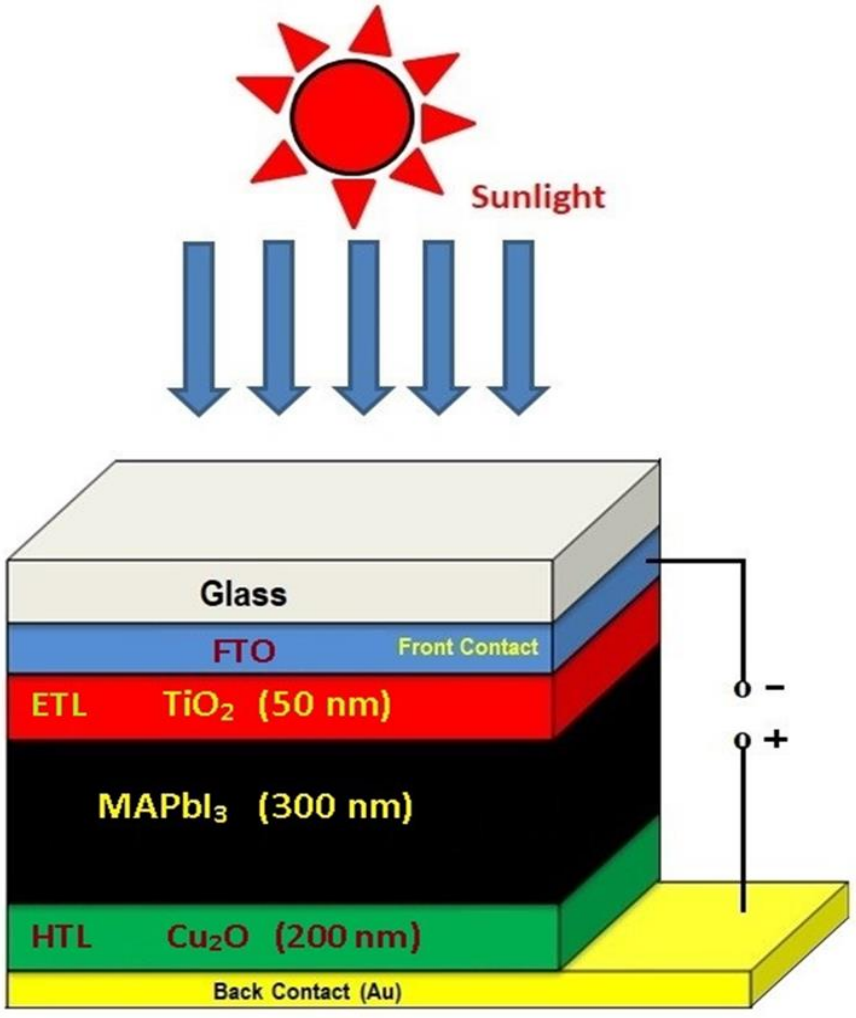

Figure 1. PSC structure and its layer parameters for COMSOL Multiphysics software.

Table 1. Component characteristics to simulate the program for COMSOL Multiphysics software (Tekin et al., 2023; Rayhan et al., 2024; Leguy et al., 2016).

Property	**Value**	**Unit**
Relative permittivity	31	1
Band gap	3[eV]	eV
Electron affinity	3.56[eV]	eV
Effective density of states, valence band	1e20[1/cm^3]	1/m³
Effective density of states, conduction band	1e20[1/cm^3]	1/m³
Electron mobility	1e-2[cm^2/(V*s)]	m²/(V·s)
Hole mobility	1e-2[cm^2/(V*s)]	m²/(V·s)
Electron lifetime, SRH	5[ns]	s
Hole lifetime, SRH	5[ns]	s

(a) ETL(TiO_2)

Property	**Value**	**Unit**
Relative permittivity	3	1
Band gap	2[eV]	eV
Electron affinity	1.9[eV]	eV
Effective density of states, valence band	1e20[1/cm^3]	1/m³
Effective density of states, conduction band	1e20[1/cm^3]	1/m³
Electron mobility	2[cm^2/(V*s)]	m²/(V·s)
Hole mobility	1e-2[cm^2/(V*s)]	m²/(V·s)
Electron lifetime, SRH	5[ns]	s
Hole lifetime, SRH	5[ns]	s

(b) HTL(Cu_2O)

Property	**Value**	**Unit**
Relative permittivity	18	1
Band gap	1.5[eV]	eV
Electron affinity	3.6[eV]	eV
Effective density of states, valence band	5e18[1/cm^3]	1/m³
Effective density of states, conduction band	5e18[1/cm^3]	1/m³
Electron mobility	2[cm^2/(V*s)]	m²/(V·s)
Hole mobility	2[cm^2/(V*s)]	m²/(V·s)
Electron lifetime, SRH	100[ns]	s
Hole lifetime, SRH	100[ns]	s

(c) PVK($MAPbI_3$)

3. Results and Discussion

The 1D simulations offer valuable insights into energy levels, carrier concentrations, and variations in electric potential, facilitating the identification of regions where charge accumulation and depletion occur, which directly impact the cell's performance. Moving to 2D simulations improves our understanding of the spatial distribution of electric fields and thermal effects, enabling us to identify areas that are prone to energy loss. Ultimately, the 3D simulations provide a more detailed perspective on these factors, allowing for a comprehensive analysis of how they influence overall device performance (Chen et al., 2021).

3.1. 1-D Simulation

Figure 2 shows the fluctuation of energy levels, carrier concentration, and electric potential in a 1D PSC as a function of arc length with their geometry. Fig. 2(a) shows the geometry in 1D for a PSC. Fig. 2(b) shows the relationship between arc length (nm) and energy (eV) illustrated in the second subfigure. The energy is constant between 0 and 50 nm of arc length, after which it rapidly rises and stabilizes. After that, the energy rises from 50 nm to 350 nm, after which it stabilizes once more. Beyond 350 nm, the energy rises continuously and at a steady rate until it reaches 550 nm. The correlation between carrier concentration ($1/cm^3$) and arc length (nm) for both electrons and holes are shown in the Fig. 2(c). From 0 to 50 nm, the electron concentration is constant; at 50 nm, it drops quickly, stabilizes momentarily, and then increases from 50 nm to 100 nm. It then decreases from 100 nm to 350 nm, stabilizes, rises from 350 nm to around 500 nm, and then decreases one more time. The concentration of holes rises from 0 to 20 nm, falls off abruptly at 50 nm, and then stabilizes. After that, it rises gradually from 50 nm to 350 nm, stabilizes, and then rises steadily further from 350 nm to 550 nm. The fluctuation of electric potential (V) with arc length (nm) is displayed in the Fig. 2(d). Between 0 and 50 nm, the electric potential is constant; between 50 and 350 nm, it decreases; and between 350 and 550 nm, it stays constant (Gu et al., 2019). Similar trends have been observed in previous studies (Kahandal et al., 2024b).

These variations are important because they provide important information about the charge transport and recombination mechanisms of the device. The energy levels and carrier concentration fluctuations show areas of charge depletion and accumulation, which have a direct impact on the PSC. In order to improve charge separation and overall PV performance, it is essential to optimize the electric field distribution within the cell, which can be achieved by understanding the electric potential profile. Design and material development for more effective PSCs can be guided by the results of this investigation (Wiktor et al., 2023).

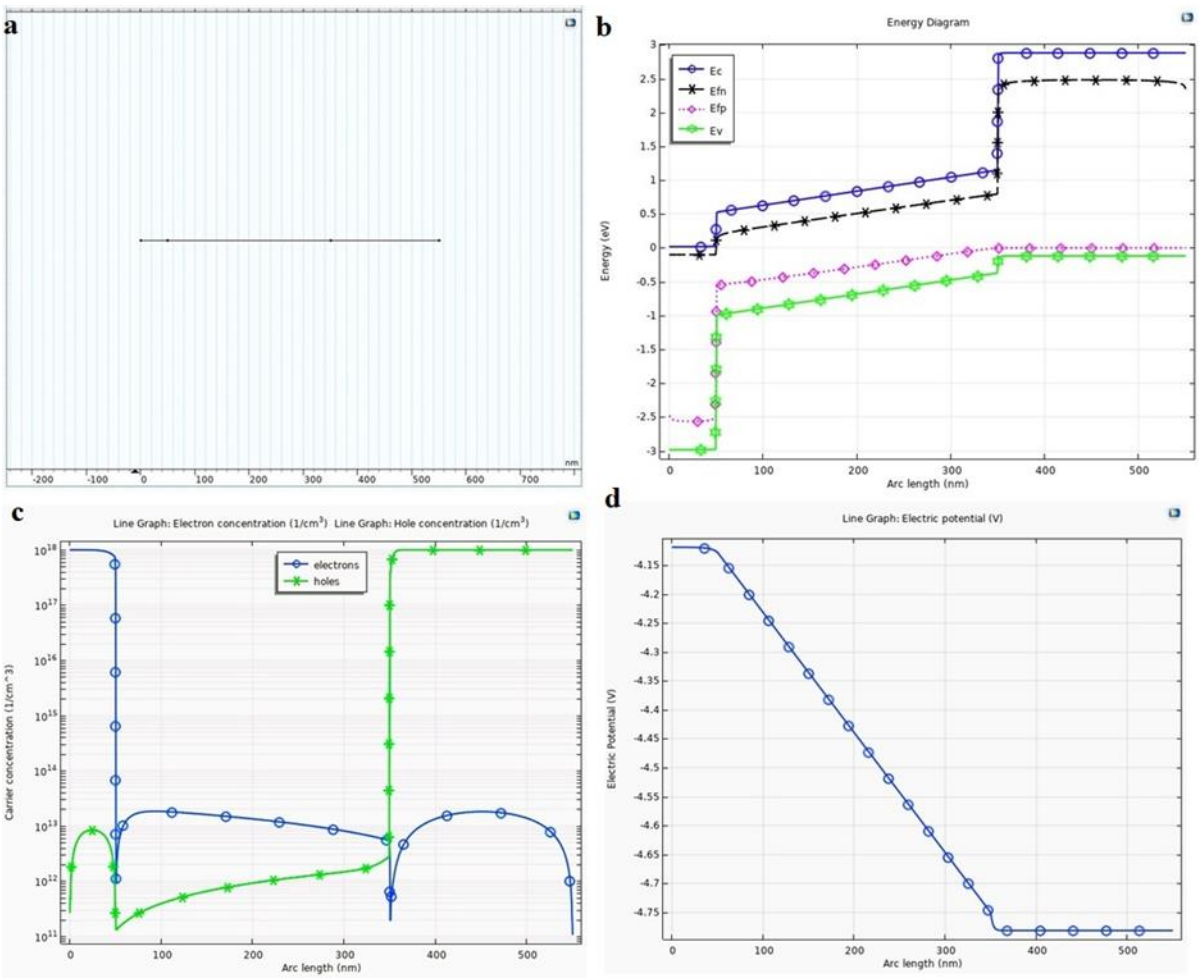

Figure 2. (a) Geometry, (b) Energy, (c) carrier concentration, and (d) electric potential vs. arc length in 1D for a PSC.

Figure 3 shows the volt-ampere (I-V) characteristic of a 1D PSC, where the relationship between applied voltage (V) and current density (mA/cm^2) is indicated. At an applied voltage of 0.01 V, the maximum current density observed is 20.8 mA/cm², showing the cell's maximal performance at this point. Beyond 0.01 V, there is a gradual decrease in the current density from 0.01 V to 1.2 V as the voltage increases (Kemmer et al., 2022). Similar trends have been observed in previous studies (Dharmadasa et al., 2019).

The I-V characteristic is important because it illustrates the peak current density of the PSC and how it decreases as voltage increases. Understanding this behavior is essential to maximizing the design for optimum power output under various operating conditions by knowing the effectiveness of the cell and its performance limitations (Kim et al., 2019).

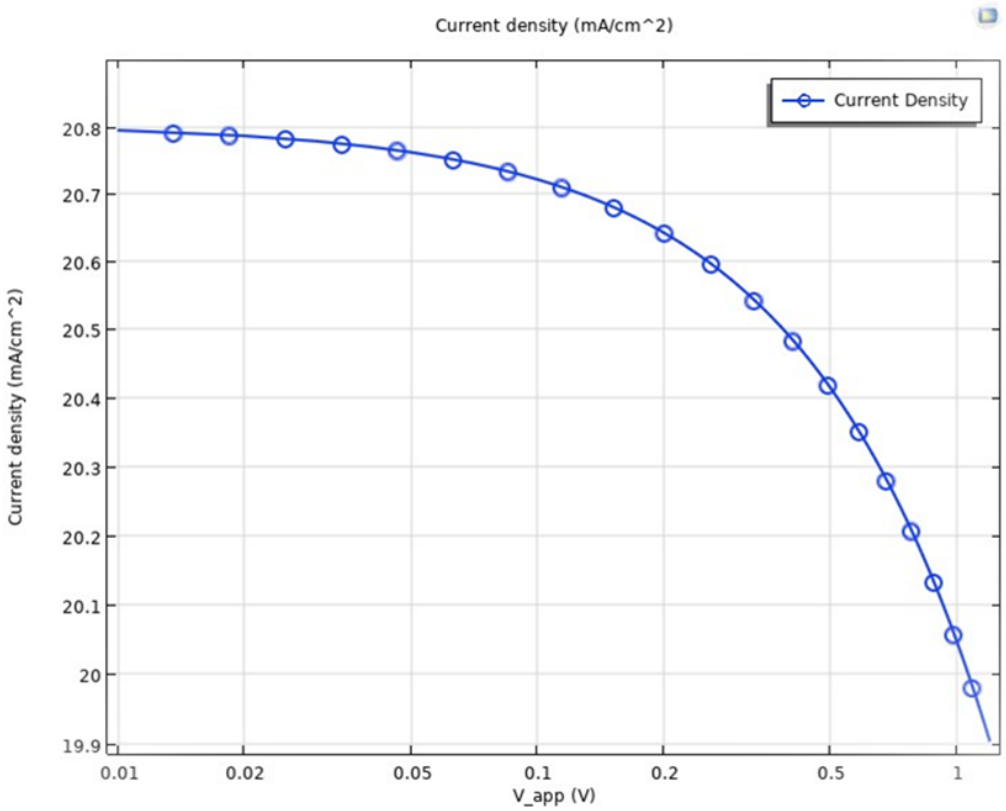

Figure 3. I-V characteristic of a PSC in 1D.

3.2. 2-D Simulation

Figure 4 shows how the electric potential, carrier concentration, and energy levels in a 2D PSC change with arc length with their geometry. Fig. 4(a) shows the geometry in 2D for a PSC. Fig. 4(b) illustrates the relationship between energy (eV) and arc length (nm). When the arc length is between 0 and 50 nm, the energy is initially constant. An energy spike occurs at 50 nm, after which it momentarily stabilizes. Once again stabilizing at 350 nm, the energy rises from 50 nm to this point. Energy increases at a constant rate beyond 350 nm and continues to do so until it reaches 550 nm. The relationship between arc length (nm) and carrier concentration ($1/cm^3$) for both electrons and holes is shown in Fig. 4(c). The concentration of electrons is constant between 0 and 50 nm, then it decreases and momentarily stabilizes at 50 nm. After this, the rate of electron concentration remains constant between 50 and 350 nm, after which it slightly decreases at 350 nm before stabilizing once more and extending steadily between 350 and 550 nm. In contrast, the concentration of holes grows and stabilizes after remaining constant between 0 and 50 nm. Beyond this, the concentration increases steadily from 50 nm to 350 nm, then increases once more at 350 nm before stabilizing and continuing at a steady pace until 550 nm. The relationship between electric potential (V) and arc length (nm) is illustrated in Fig. 4(d). Between 0 and 50 nm, the electric potential is constant. After that, it starts decreasing and gradually stabilizes. The potential

keeps going at a steady pace from 50 nm to 350 nm and then stays constant up to 550 nm beyond this (Steele et al., 2023).

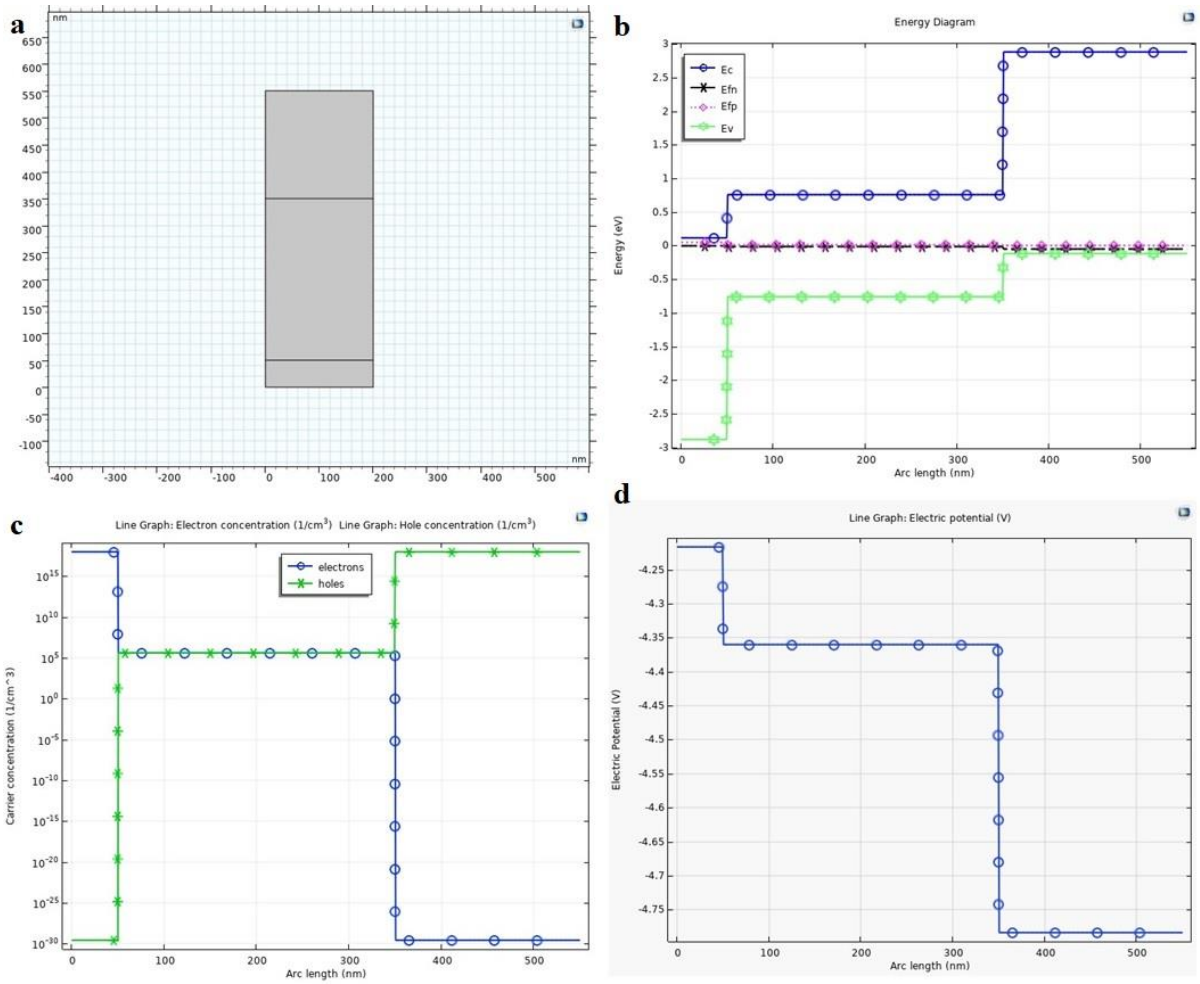

Figure 4. (a) Geometry, (b) Energy, (c) carrier concentration, and (d) electric potential vs. arc length in 2D for a PSC.

This relation is crucial because it shows in great detail how the electric potential, carrier concentration, and energy levels in a 2D PSC change over the arc length. Understanding the internal charge transport dynamics and potential distribution within the cell, which have a direct effect on its performance and effectiveness, requires a comprehension of these variances. Through the examination of these profiles, scientists can find crucial areas that may witness charge accumulation, recombination, or other obstructions. This information can then be utilized to influence the improvement of material characteristics and device architecture, ultimately enhancing the total effectiveness of solar cells (Smith & Karaman, 2019).

Figure 5 shows a complete 2D illustration of the electric field norm, nonradiative recombination heating, total heat source, and joule heating in a PSC operating at 1.2 V. The hot side of the simulation of the electric field norm (V/m) in Fig. 5(a) reaches a value of 9.64×10^{6} V/m, while the cold side is much lower at 1.03×10^{3} V/m. This indicates a large spatial variation in

the electric field within the cell. With a hot side value of -3.46×10⁸ W/m³ and a cold side value of -1.47×10⁹ W/m³, Fig. 5(b) illustrates the simulation of nonradiative recombination heating (W/m³) and highlights the areas where energy loss from nonradiative processes occurs. The simulation of the total heat source (W/m³) is shown in Fig. 5(c), where the hot side value is 3.63×10⁸ W/m³ and the cold side value is -1.47×10⁹ W/m³. This represents all of the heating sources in the cell, both radiative and nonradiative. In Fig. 5(c), the simulation of joule heating (W/m³) is shown. The resistive losses within the device are reflected by the hot side, which reaches a value of 1.84×10⁹ W/m³, and the cool side, which is substantially lower at 1.99×10⁵ W/m³. In order to comprehend the mechanisms influencing the stability and performance of the PSC, it is imperative to have a thorough understanding of the thermal and electrical behavior of the device (Li et al., 2021). Similar trends have been observed in previous studies (Zhou et al., 2024; Deceglie et al., 2012).

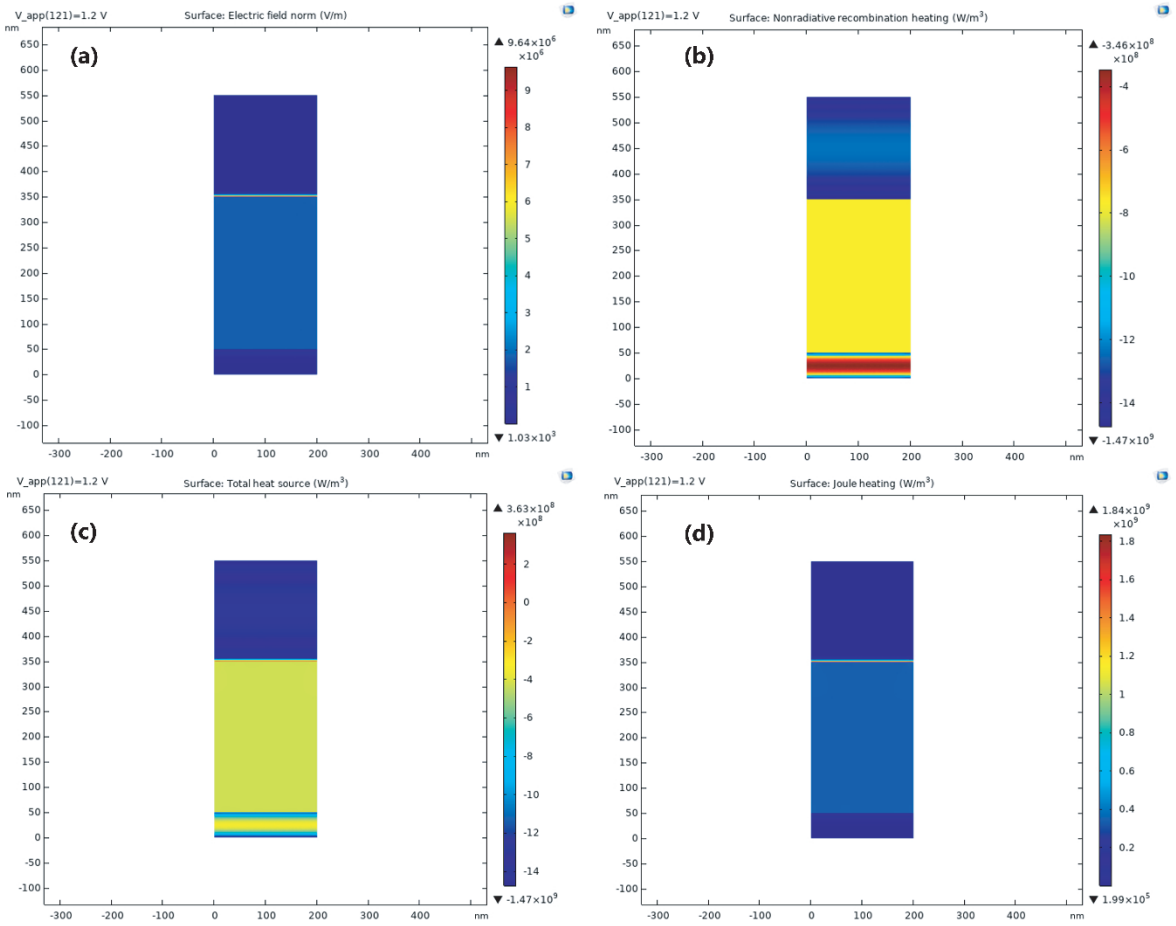

Figure 5. 2D representation combining (a) electric field norm, (b) nonradiative recombination heating, (c) total heat source, and (d) joule heating in a PSC.

This simulation is important because it shows how the electric field, heat production, and dissipation processes are distributed spatially in a PSC when 1.2 V of applied voltage is used. It is essential to comprehend the differences in the electric field norm, nonradiative recombination heating, total heat source, and joule heating across the cell in order to pinpoint areas of energy loss

and enhance the device's thermal and electrical performance. This realization is crucial for raising PSCs effectiveness and long-term stability (Yuan et al., 2019).

3.3. 3-D Simulation

In Figure 6, energy, carrier concentration, and electric potential in a PSC are shown in 3D as functions of arc length, exhibiting the behavior shown in Figure 4 in a similar way. Along the arc length, energy and electric potential exhibit consistent variations, whereas carrier concentration demonstrates matching changes for electrons and holes. The energy and carrier concentrations also exhibit comparable trends.

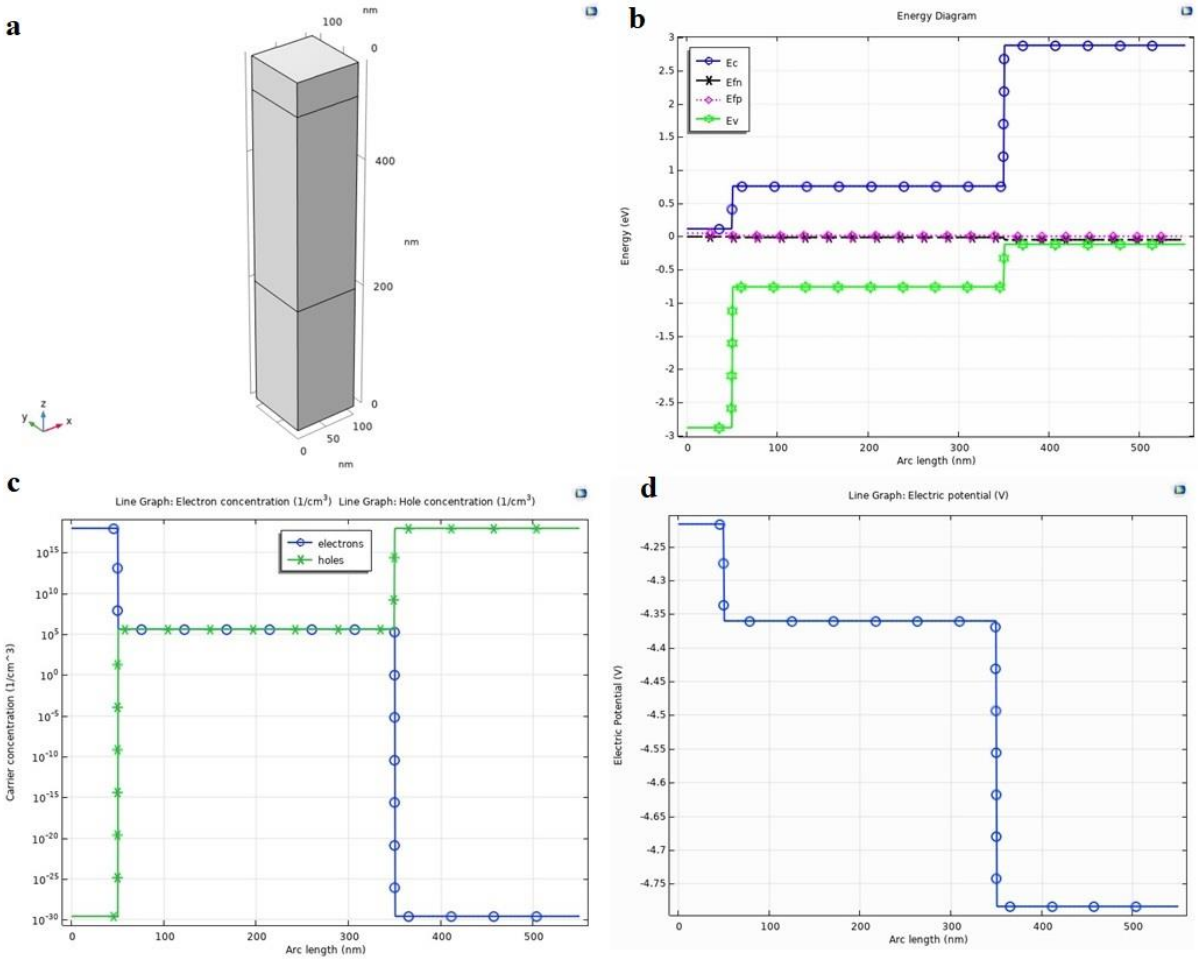

Figure 6. (a) Geometry, (b) Energy, (c) carrier concentration, and (d) electric potential vs. arc length in 2D for a PSC.

4. Conclusion

In this research, COMSOL Multiphysics was employed to perform a comprehensive simulation analysis of perovskite solar cells (PSCs) in 1-D, 2-D, and 3-D configurations, providing valuable insights into the spatial distribution of their electrical and thermal properties. Understanding these properties is key to improving device performance. The 1-D simulations

revealed the interconnections between energy levels, carrier concentrations, and electric potential, which directly influence overall cell performance. The I-V characteristics demonstrated the importance of applied voltage in achieving maximum current density and power output. In the 2-D simulations, the analysis extended to include variations in electric fields, nonradiative recombination heating, total heat sources, and joule heating, underscoring the significance of thermal management and charge transport mechanisms in enhancing cell stability and performance. By identifying areas of energy loss and thermal accumulation, we highlighted opportunities for improving material properties and device architecture. The 3-D simulations, building on the 2-D results, provided a more detailed spatial perspective. Overall, our research demonstrates the effectiveness of using multidimensional simulations to comprehensively understand PSC behaviour. The findings highlight the importance of optimal material properties, device structure, and thermal management to achieve higher performance and stability in PSCs. Future research could focus on experimentally validating these simulation results and exploring advanced materials and designs to further enhance PSC performance.

Declaration of Competing Interest

There are no competing interests between the authors and the publication of this article. Furthermore, no other journal has previously published this research.

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References

Ball, James M., Michael M. Lee, Andrew Hey, & Henry J. Snaith. (2013). "Low-Temperature Processed Meso-Superstructured to Thin-Film Perovskite Solar Cells." *Energy and Environmental Science.* 6(6): 1739–43. doi:10.1039/c3ee40810h.

Bati, Abdulaziz S.R., Yu Lin Zhong, Paul L. Burn, Mohammad Khaja Nazeeruddin, Paul E. Shaw, & Munkhbayar Batmunkh. (2023). "Next-Generation Applications for Integrated Perovskite Solar Cells." *Communications Materials.* 4(1): 1–24. doi:10.1038/s43246-022-00325-4.

Bi, Dongqin, Chenyi Yi, Jingshan Luo, Jean David Décoppet, Fei Zhang, Shaik Mohammed Zakeeruddin, Xiong Li, Anders Hagfeldt, & Michael Grätzel. (2016). "Polymer-Templated Nucleation and Crystal Growth of Perovskite Films for Solar Cells with Efficiency Greater than 21%." *Nature Energy.* 1(10): 1–5. doi:10.1038/nenergy.2016.142.

Brenner, Thomas M., David A. Egger, Leeor Kronik, Gary Hodes, & David Cahen. (2016). "Hybrid Organic - Inorganic Perovskites: Low-Cost Semiconductors with Intriguing Charge-Transport Properties." *Nature Reviews Materials.* 1(1): 1–16. doi:10.1038/natrevmats.2015.7.

Burschka, Julian, Norman Pellet, Soo Jin Moon, Robin Humphry-Baker, Peng Gao, Mohammad K. Nazeeruddin, & Michael Grätzel. (2013). "Sequential Deposition as a Route to High-Performance Perovskite-Sensitized Solar Cells." *Nature.* 499(7458): 316–19. doi:10.1038/nature12340.

Chen, Wei Hsin, Bo Jhih Lin, Yu Ying Lin, Yen Shih Chu, Aristotle T. Ubando, Pau Loke Show,& Hwai Chyuan Ong, et al. (2021). "Progress in Biomass Torrefaction: Principles, Applications and Challenges." *Progress in Energy and Combustion Science.* 82: 100887. doi:10.1016/j.pecs.2020.100887.

Conings, Bert, Jeroen Drijkoningen, Nicolas Gauquelin, Aslihan Babayigit, Jan D'Haen, Lien D'Olieslaeger,& Anitha Ethirajan, et al. (2015). "Intrinsic Thermal Instability of Methylammonium Lead Trihalide Perovskite." *Advanced Energy Materials.* 5(15). doi:10.1002/aenm.201500477.

Deceglie, Michael G., Vivian E. Ferry, A. Paul Alivisatos, & Harry A. Atwater. (2012). "Design of Nanostructured Solar Cells Using Coupled Optical and Electrical Modeling." *Nano Letters.* 12(6): 2894–2900. doi:10.1021/nl300483y.

Dharmadasa, I. M., Y. Rahaq, A. A. Ojo, & T. I. Alanazi. (2019). "Perovskite Solar Cells: A Deep Analysis Using Current–Voltage and Capacitance–Voltage Techniques." *Journal of Materials Science: Materials in Electronics.* 30(2): 1227–35. doi:10.1007/s10854-018-0390-5.

Eperon, Giles E., Samuel D. Stranks, Christopher Menelaou, Michael B. Johnston, Laura M. Herz, & Henry J. Snaith. (2014). "Formamidinium Lead Trihalide: A Broadly Tunable Perovskite for Efficient Planar Heterojunction Solar Cells." *Energy and Environmental Science.* 7(3): 982–88. doi:10.1039/c3ee43822h.

Green, Martin A., Ewan D. Dunlop, Masahiro Yoshita, Nikos Kopidakis, Karsten Bothe, Gerald Siefer, & Xiaojing Hao. (2024). "Solar Cell Efficiency Tables (Version 63)." *Progress in Photovoltaics: Research and Applications.* 32(1): 3–13. doi:10.1002/pip.3750.

Gu, Hao, Chao Liang, Yingdong Xia, Qi Wei, Tanghao Liu, Yingguo Yang, & Wei Hui, et al. (2019). "Nanoscale Hybrid Multidimensional Perovskites with Alternating Cations for High Performance Photovoltaic." *Nano Energy.* 65(May): 104050. doi:10.1016/j.nanoen.2019.104050.

Habisreutinger, Severin N., Tomas Leijtens, Giles E. Eperon, Samuel D. Stranks, Robin J. Nicholas, & Henry J. Snaith. (2014). "Carbon Nanotube/Polymer Composites as a Highly Stable Hole Collection Layer in Perovskite Solar Cells." *Nano Letters.* 14(10): 5561–68. doi:10.1021/nl501982b.

Hägglund, & Carl. (2022). "Multiscale Optical Modeling of Perovskite-Si Tandem Solar Cells." *Frontiers in Photonics.* 3(July): 1–15. doi:10.3389/fphot.2022.921438.

Im, Jeong Hyeok, Hui Seon Kim, & Nam Gyu Park. (2014). "Morphology-Photovoltaic Property

Correlation in Perovskite Solar Cells: One-Step versus Two-Step Deposition of CH3NH3PbI 3." *APL Materials.* 2(8). doi:10.1063/1.4891275.

Jeon, Nam Joong, Jun Hong Noh, Young Chan Kim, Woon Seok Yang, Seungchan Ryu, & Sang Il Seok. (2014). "Solvent Engineering for High-Performance Inorganic-Organic Hybrid Perovskite Solar Cells." *Nature Materials.* 13(9): 897–903. doi:10.1038/nmat4014.

Jiang, Yunmeng, Yanhua Cheng, Shunjie Liu, Haoke Zhang, Xiaoyan Zheng, Ming Chen, Michidmaa & Khorloo, et al. (2021). "Solid-State Intramolecular Motions in Continuous Fibers Driven by Ambient Humidity for Fluorescent Sensors." *National Science Review.* 8(4). doi:10.1093/nsr/nwaa135.

Kahandal, Suman S., Rameshwar S. Tupke, Dinesh S. Bobade, Hansol Kim, Guanghai Piao, Babasaheb R. Sankapal, & Zafar Said, et al. (2024a). "Perovskite Solar Cells: Fundamental Aspects, Stability Challenges, and Future Prospects." *Progress in Solid State Chemistry.* 74: 100463. doi:10.1016/J.PROGSOLIDSTCHEM.2024.100463.

Kahandal, Suman S., Rameshwar S. Tupke, Dinesh S. Bobade, Hansol Kim, Guanghai Piao, Babasaheb R. Sankapal, & Zafar Said, et al. (2024b). "Perovskite Solar Cells: Fundamental Aspects, Stability Challenges, and Future Prospects." *Progress in Solid State Chemistry.* 74: 100463. doi:10.1016/J.PROGSOLIDSTCHEM.2024.100463.

Kemmer, Tobias, Johannes M. Greulich, Alexander Krieg, & Stefan Rein. (2022). "Current-Voltage Characteristics of Silicon Solar Cells: Determination of Base Doping Concentration and Hysteresis Correction." *Solar Energy Materials and Solar Cells.* 248: 111953. doi:10.1016/J.SOLMAT.2022.111953.

Khan, Aryan Dilawar, Muhammad Mustajab, Sawaira Moeen, Muhammad Imran, Muhammad Ikram, Qasim Khan, & Maaz Khan. (2024). "Advancements in the Stability, Protection and Lead-Free Strategies of Perovskite Solar Cells: A Critical Review." *Environmental Science: Advances.* 3(7): 1004–29. doi:10.1039/d3va00401e.

Kim, Eun Bi, M. Shaheer Akhtar, Hyung Shik Shin, Sadia Ameen, & Mohammad Khaja Nazeeruddin. (2021). "A Review on Two-Dimensional (2D) and 2D-3D Multidimensional Perovskite Solar Cells: Perovskites Structures, Stability, and Photovoltaic Performances." *Journal of Photochemistry and Photobiology C: Photochemistry Reviews.* 48(February): 100405. doi:10.1016/j.jphotochemrev.2021.100405.

Kim, Minjin, Gi Hwan Kim, Tae Kyung Lee, In Woo Choi, Hye Won Choi, Yimhyun Jo, & Yung Jin Yoon, et al. (2019). "Methylammonium Chloride Induces Intermediate Phase Stabilization for Efficient Perovskite Solar Cells." *Joule.* 3(9): 2179–92. doi:10.1016/j.joule.2019.06.014.

Kojima, Akihiro, Kenjiro Teshima, Yasuo Shirai, & Tsutomu Miyasaka. (2009). "Organometal Halide Perovskites as Visible-Light Sensitizers for Photovoltaic." : 6050–51.

Kumar, Anirudh, Deepak Kumar, Naini Jain, Manoj Kumar, Gajanan Ghodake, Sushil Kumar, & Rupendra K. Sharma, et al. (2023). "Enhanced Efficiency and Stability of Electron Transport Layer in Perovskite Tandem Solar Cells: Challenges and Future Perspectives." *Solar Energy*. 266: 112185. doi:10.1016/J.SOLENER.2023.112185.

Kumar, Anjan, Sangeeta Singh, Mustafa K.A. Mohammed, & Ahmed Esmail Shalan. (2021). "Effect of 2D Perovskite Layer and Multivalent Defect on the Performance of 3D/2D Bilayered Perovskite Solar Cells through Computational Simulation Studies." *Solar Energy*. 223(March): 193–201. doi:10.1016/j.solener.2021.05.042.

Kumar, Naveen, Raju Kannadasan, B B Beenarani, Mohammed H Alsharif, Mun-kyeom Kim, & Z Hasan Inamul. (2024). "Recent Developments in Perovskite Materials , Fabrication Techniques , Band Gap Engineering , and the Stability of Perovskite Solar Cells." *Energy Reports*. 11(December 2023): 1171–90. doi:10.1016/j.egyr.2023.12.068.

Leguy, Aurélien M.A., Pooya Azarhoosh, M. Isabel Alonso, Mariano Campoy-Quiles, Oliver J. Weber, Jizhong Yao, & Daniel Bryant, et al. (2016). "Experimental and Theoretical Optical Properties of Methylammonium Lead Halide Perovskites." *Nanoscale*. 8(12): 6317–27. doi:10.1039/c5nr05435d.

Li, Peixian, Xuyan Yan, Shuiying Gao, & Rong Cao. (2021). "Boosting Photocatalytic Hydrogen Production Coupled with Benzyl Alcohol Oxidation over CdS/Metal–Organic Framework Composites." *Chemical Engineering Journal*. 421(P1): 129870. doi:10.1016/j.cej.2021.129870.

Li, Xin, Sikandar Aftab, Sajjad Hussain, Fahmid Kabir, A. M.A. Henaish, Abdullah G. Al-Sehemi, Mohan Reddy Pallavolu, & Ganesh Koyyada. (2024). "Dimensional Diversity (0D, 1D, 2D, and 3D) in Perovskite Solar Cells: Exploring the Potential of Mixed-Dimensional Integrations." *Journal of Materials Chemistry A*. 12(8): 4421–40. doi:10.1039/d3ta06953b.

Li, Zhiqiang, Xiaoyang Liang, Gang Li, Haixu Liu, Huiyu Zhang, Jianxin Guo, & Jingwei Chen, et al. (2019). "9.2%-Efficient Core-Shell Structured Antimony Selenide Nanorod Array Solar Cells." *Nature Communications*. 10(1): 1–9. doi:10.1038/s41467-018-07903-6.

Lin, Yuze, Liang Shen, Jun Dai, Yehao Deng, Yang Wu, Yang Bai, & Xiaopeng Zheng, et al. (2017). "π-Conjugated Lewis Base: Efficient Trap-Passivation and Charge-Extraction for Hybrid Perovskite Solar Cells." *Advanced Materials*. 29(7). doi:10.1002/adma.201604545.

Liu, Guo, Xiaofeng Zhang, Xuliang Chen, Yunhu He, Lizi Cheng, Mengke Huo, & Jianan Yin, et al. (2021). "Materials Science & Engineering R Additive Manufacturing of Structural Materials." *Materials Science & Engineering*. R (xxxx): 100596. doi:10.1016/j.mser.2020.100596.

Liu, Yucheng, Haochen Ye, Yunxia Zhang, Kui Zhao, Zhou Yang, Yongbo Yuan, & Haodi Wu, et al. (2019). "Surface-Tension-Controlled Crystallization for High-Quality 2D Perovskite

Single Crystals for Ultrahigh Photodetection." *Matter.* 1(2): 465–80. doi:10.1016/j.matt.2019.04.002.

Minbashi, Mehran, & Elnaz Yazdani. (2022). "Comprehensive Study of Anomalous Hysteresis Behavior in Perovskite-Based Solar Cells." *Scientific Reports.* 12(1): 1–14. doi:10.1038/s41598-022-19194-5.

Niu, Guangda, Xudong Guo, & Liduo Wang. (2015). "Review of Recent Progress in Chemical Stability of Perovskite Solar Cells." *Journal of Materials Chemistry A.* 3(17): 8970–80. doi:10.1039/c4ta04994b.

Rao, Maithili K, D N Sangeetha, M Selvakumar, Y N Sudhakar, & M G Mahesha. (2021). "Review on Persistent Challenges of Perovskite Solar Cells ' Stability." *Solar Energy.* 218(February): 469–91. doi:10.1016/j.solener.2021.03.005.

Rayhan, Abu, M. A. Khan, & Md Rabiul Islam. (2024). "Enhancing CsSn0.5Ge0.5I3 Perovskite Solar Cell Performance via Cu2O Hole Transport Layer Integration." *International Journal of Photoenergy.* 2024(I). doi:10.1155/2024/8859153.

Rehman, Waqaas, David P. McMeekin, Jay B. Patel, Rebecca L. Milot, Michael B. Johnston, Henry J. Snaith, & Laura M. Herz. (2017). "Photovoltaic Mixed-Cation Lead Mixed-Halide Perovskites: Links between Crystallinity, Photo-Stability and Electronic Properties." *Energy and Environmental Science.* 10(1): 361–69. doi:10.1039/c6ee03014a.

Saxena, Prateek, & Nima E. Gorji. (2019). "COMSOL Simulation of Heat Distribution in Perovskite Solar Cells: Coupled Optical-Electrical-Thermal 3-D Analysis." *IEEE Journal of Photovoltaics.* 9(6): 1693–98. doi:10.1109/JPHOTOV.2019.2940886.

Seo, You Hyun, Eun Chong Kim, Se Phin Cho, Seok Soon Kim, & Seok In Na. (2017). "High-Performance Planar Perovskite Solar Cells: Influence of Solvent upon Performance." *Applied Materials Today.* 9: 598–604. doi:10.1016/J.APMT.2017.11.003.

Smith, Robert, & Mehmet Akif Karaman. (2019). "Development and Validation of the Contextual Achievement Motivation Measure." *International Journal of Psychology and Educational Studies.* 6(3): 16–26. doi:10.17220/ijpes.2019.03.003.

Snaith, & Henry J. (2013). "Perovskites: The Emergence of a New Era for Low-Cost, High-Efficiency Solar Cells." *Journal of Physical Chemistry Letters.* 4(21): 3623–30. doi:10.1021/jz4020162.

Song, Guang Hua, & Hua Meng. (2013). "Numerical Modeling and Simulation of PEM Fuel Cells: Progress and Perspective." *Acta Mechanica Sinica/Lixue Xuebao.* 29(3): 318–34. doi:10.1007/s10409-013-0037-y.

Steele, Andrew D., Alexander F. Kiefer, & Ben Shen. (2023). "The Many Facets of Sulfur Incorporation in Natural Product Biosynthesis." *Current Opinion in Chemical Biology.* 76: 102366. doi:10.1016/J.CBPA.2023.102366.

Stranks, Samuel D., Giles E. Eperon, Giulia Grancini, Christopher Menelaou, Marcelo J.P. Alcocer, Tomas Leijtens, Laura M. Herz, Annamaria Petrozza, & Henry J. Snaith. (2013). "Electron-Hole Diffusion Lengths Exceeding 1 Micrometer in an Organometal Trihalide Perovskite Absorber." *Science.* 342(6156): 341–44. doi:10.1126/science.1243982.

Targhi, Farhad Fouladi, Yousef Seyed Jalili, & Faramarz Kanjouri. (2018). "MAPbI3 and FAPbI3 Perovskites as Solar Cells: Case Study on Structural, Electrical and Optical Properties." *Results in Physics.* 10(May): 616–27. doi:10.1016/j.rinp.2018.07.007.

Tekin, S. B., S. Almalki, H. Finch, A. Vezzoli, L. O'Brien, V. R. Dhanak, S. Hall, & I. Z. Mitrovic. (2023). "Electron Affinity of Metal Oxide Thin Films of TiO2, ZnO, and NiO and Their Applicability in 28.3 THz Rectenna Devices." *Journal of Applied Physics.* 134(8). doi:10.1063/5.0157726.

Wang, Haoran, Xiwen Gong, Dewei Zhao, Yong Biao Zhao, Sheng Wang, Jianfeng Zhang, & Lingmei Kong, et al. (2020). "A Multi-Functional Molecular Modifier Enabling Efficient Large-Area Perovskite Light-Emitting Diodes." *Joule.* 4(9): 1977–87. doi:10.1016/j.joule.2020.07.002.

Wiktor, Julia, Erik Fransson, Dominik Kubicki, & Paul Erhart. (2023). "Quantifying Dynamic Tilting in Halide Perovskites: Chemical Trends and Local Correlations." *Chemistry of Materials.* 35(17): 6737–44. doi:10.1021/acs.chemmater.3c00933.

Wu, Wu Qiang, Qi Wang, Yanjun Fang, Yuchuan Shao, Shi Tang, Yehao Deng, & Haidong Lu, et al. (2018). "Molecular Doping Enabled Scalable Blading of Efficient Hole-Transport-Layer-Free Perovskite Solar Cells." *Nature Communications.* 9(1): 1–8. doi:10.1038/s41467-018-04028-8.

Yamaguchi, Masafumi, Frank Dimroth, John F. Geisz, & Nicholas J. Ekins-Daukes. (2021). "Multi-Junction Solar Cells Paving the Way for Super High-Efficiency." *Journal of Applied Physics.* 129(24). doi:10.1063/5.0048653.

Yang, Zhibin, Adharsh Rajagopal, Chu Chen Chueh, Sae Byeok Jo, Bo Liu, Ting Zhao, & Alex K.Y. Jen. (2016). "Stable Low-Bandgap Pb–Sn Binary Perovskites for Tandem Solar Cells." *Advanced Materials.* 28(40): 8990–97. doi:10.1002/adma.201602696.

Yao, Liquan, Limei Lin, Hui Liu, Fengying Wu, Jianmin Li, Shuiyuan Chen, Zhigao Huang, & Guilin Chen. (2020). "Front and Back Contact Engineering for High-Efficient and Low-Cost Hydrothermal Derived Sb2(S, Se)3 Solar Cells by Using FTO/SnO2 and Carbon." *Journal of Materials Science and Technology.* 58: 130–37. doi:10.1016/j.jmst.2020.03.049.

Yuan, Jun, Yunqiang Zhang, Liuyang Zhou, Guichuan Zhang, Hin Lap Yip, Tsz Ki Lau, & Xinhui Lu, et al. (2019). "Single-Junction Organic Solar Cell with over 15% Efficiency Using Fused-Ring Acceptor with Electron-Deficient Core." *Joule.* 3(4): 1140–51. doi:10.1016/j.joule.2019.01.004.

Zandi, Soma, Prateek Saxena, & Nima E Gorji. (2020). "Numerical Simulation of Heat Distribution in RGO-Contacted Perovskite Solar Cells Using COMSOL." *Solar Energy.* 197(December 2019): 105–10. doi:10.1016/j.solener.2019.12.050.

Zhang, Huiyin, Yiming Li, Shan Tan, Zijing Chen, Keke Song, Shixian Huang, & Jiangjian Shi, et al. (2022). "High-Efficiency (>20%) Planar Carbon-Based Perovskite Solar Cells through Device Configuration Engineering." *Journal of Colloid and Interface Science.* 608: 3151–58. doi:10.1016/J.JCIS.2021.11.050.

Zhao, Chang Xin, Jia Ning Liu, Bo Quan Li, Ding Ren, Xiao Chen, Jia Yu, & Qiang Zhang. (2020). "Multiscale Construction of Bifunctional Electrocatalysts for Long-Lifespan Rechargeable Zinc–Air Batteries." *Advanced Functional Materials.* 30(36): 1–9. doi:10.1002/adfm.202003619.

Zhou, Miao, Zhengang Guo, & Zhifeng Liu. (2020). "FeOOH as Hole Transfer Layer to Retard the Photocorrosion of Cu2O for Enhanced Photoelctrochemical Performance." *Applied Catalysis B: Environmental.* 260: 118213. doi:10.1016/j.apcatb.2019.118213.

Zhou, Qingwei, Jialong Duan, Jian Du, Qiyao Guo, Qiaoyu Zhang, Xiya Yang, Yanyan Duan, & Qunwei Tang. (2021). "Tailored Lattice 'Tape' to Confine Tensile Interface for 11.08%-Efficiency All-Inorganic CsPbBr3 Perovskite Solar Cell with an Ultrahigh Voltage of 1.702 V." *Advanced Science.* 8(19): 1–9. doi:10.1002/advs.202101418.

Zhou, Tingxue, Xin Huang, Diao Zhang, Wei Liu, & Xing'ao Li. (2024). "Design and Simulation for Minimizing Non-Radiative Recombination Losses in CsGeI2Br Perovskite Solar Cells." *Nanomaterials.* 14(20): 1–10. doi:10.3390/nano14201650.